

# Metamagnetic phase transition in the Ising plus Dzyaloshinskii-Moriya model

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We study the 1D ferromagnetic Ising (spin-1/2) model with the Dzyaloshinskii-Moriya (DM) interaction. We analyze the low energy excitation spectrum and the ground state magnetic phase diagram using the Lanczos method. The DM interaction-dependency is calculated for the low-energy excitation spectrum, spiral order parameter and spin-spin correlation functions. We show that a metamagnetic quantum phase transition occurs between the ferromagnetic and spiral phases. The existence of the metamagnetic phase transition is confirmed, using the variational matrix product states approach.

PACS numbers: 75.10.Jm Quantized spin models; 75.10.Pq Spin chain models

## I. INTRODUCTION

Studying one dimensional quantum spin systems have been obtained many interesting results. The Ising spin models pose intriguing theoretical problems because antiferromagnetic (AF) and ferromagnetic (FM) systems with spin-1/2 have a gap in the excitation spectrum. Therefore they reveal an extremely rich behavior dominated by quantum effects. In particular, the spin-1/2 Ising model in a transverse magnetic field (ITF) displays a pragmatic example of a quantum phase transition. Theoretically, the ITF problem is exactly solved<sup>1</sup> and found a phase transition at a finite value of the transverse magnetic field:  $h_c$ . This is a quantum critical point and the phase transition is continuous in nature.

The antisymmetric spin exchange interactions between spins, known as the Dzyaloshinskii-Moriya (DM) interaction, play an important role in physics of spin systems<sup>2,3</sup>. The DM interaction idea originated from the deviation of experimental data from the theoretical predictions, based on the Heisenberg spin Hamiltonians<sup>4,5,6,7,8,9,10,11,12</sup>. Generally the DM interaction between two spins  $S_1, S_2$  can be written as  $\mathbf{D} \cdot (\mathbf{S}_1 \times \mathbf{S}_2)$  with an axial DM vector  $\mathbf{D}$ . In actual systems, the direction of  $\mathbf{D}$  vector is fixed by the microscopic arrangement of atoms and orbitals. In a spin chain, the DM vector may vary both in direction and magnitude. However, the symmetry arguments usually rule out most of possibilities and confine the theoretical discussion to two principal cases. The first one is the uniform DM interaction,  $\mathbf{D} = \text{constant}$  over the system<sup>13</sup> and the second case is the staggered DM interaction<sup>14</sup> with anti-parallel  $\mathbf{D}$  on adjacent bonds. Since the DM interaction is rather difficult to handle analytically, the effect of this interaction are only partially studied so far. In this sense we study the Ising chain (FM) with DM interaction, that its Hamiltonian (by considering a periodic

chain of  $N$  sites) is given by

$$\mathcal{H} = J \sum_j S_j^z S_{j+1}^z + \sum_j \mathbf{D} \cdot (\mathbf{S}_j \times \mathbf{S}_{j+1}), \quad (1)$$

where  $\mathbf{S}_j$  is spin-1/2 operator on the  $j$ -th site, and  $J > 0$  ( $J < 0$ ) denotes the AF (FM) coupling constant. In a very recent work, using the quantum renormalization group and numerical Lanczos methods, the ground state phase diagram of the AF Ising chain ( $J > 0$ ) is studied<sup>15</sup>. It is shown that the ground state phase diagram consists of AF and spiral phases.

By considering uniform DM vector as  $\mathbf{D} = D\hat{z}$ , and doing the rotation about  $z$  axis as  $S_j^\pm \rightarrow S_j^\pm e^{\pm i\frac{j\pi}{2}}$ , the Hamiltonian is transformed to XXZ chain<sup>16,17</sup> with an anisotropy parameter  $\frac{J}{D}$ , i.e.,

$$\mathcal{H}^{tr} = D \sum_j \left[ (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \frac{J}{D} S_j^z S_{j+1}^z \right]. \quad (2)$$

The XXZ chain model was solved by Bethe<sup>18</sup>, and its ground state phase diagram is well known<sup>19</sup>. The Neel regime is governed by  $\frac{J}{D} > 1$  and there is a gap in the excitation spectrum. For  $\frac{J}{D} \leq -1$ , the ground state is in the FM phase and there is a gap over the FM state. In the region  $-1 < \frac{J}{D} \leq 1$ , the ground state of the system is in the gapless Luttinger liquid (LL) phase. Thus, by increasing the  $D$  value, the system undergoes a quantum phase transition from the gapped Neel (or FM) phase to the gapless LL phase at the critical value  $D_c = J$ .

In this paper we study an Ising spin-1/2 chain with FM exchange ( $J < 0$ ) and the uniform DM interaction using the numerical and analytical approaches. In the forthcoming section, we apply the Lanczos method to diagonalize numerically finite chain systems with lengths  $N = 8, 10, \dots, 24$ . Using the exact diagonalization results, we calculate the spin gap, magnetization and spin-spin correlations as a function of the DM interaction. We

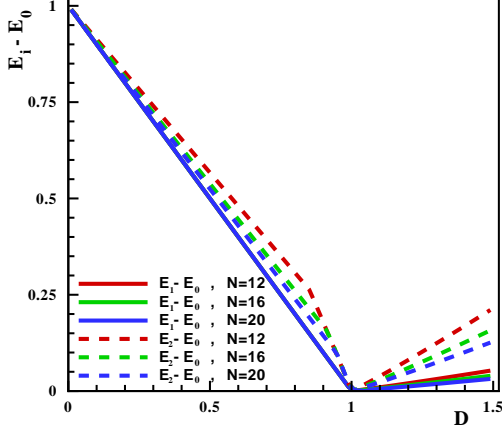


FIG. 1: Difference between the energy of the two lowest levels and the ground state energy as a function of the DM vector, for chains with FM exchange ( $J = -1.0$ ) including different lengths  $N = 12, 16, 20$ .

have also calculated the spirality in the ground state of the system. Based on the exact diagonalization results we obtain the ground-state magnetic phase diagram of the model. By taking the DM interaction as the control parameter we show that a metamagnetic phase transition, can be observed in the 1D ferromagnetic Ising model. In section III, the observed metamagnetic phase transition from the numerical lanczos method is confirmed by the analyzing the results of the variational matrix product states approach. Finally, we conclude and summarize our results in section IV.

## II. NUMERICAL RESULTS

In this section, to explore the nature of the spectrum and the quantum phase transition, we use the Lanczos method to diagonalize chains with length up to  $N = 24$ . We have computed the three lowest energy eigenvalues of chains with FM exchange  $J = -1.0$  and different values of the DM vector. To get the energies of the few lowest eigenstates we consider chains with periodic boundary conditions. In Fig.1, we have presented results of these calculations for the chain sizes  $N = 12, 16, 20$ . We define the excitation gap as a gap to the first excited state. It exhibits that the energy spectrum is gapped at  $D = 0$ , while by increasing the  $D$  the energy gap decreases linearly and vanishes at  $D_c = |J| = 1.0$ . We got this critical value as an exact value since there was no finite size correction. In the region  $D < D_c$ , the difference between the energy of the first excited state and the ground state energy shows an universal linear decrease with increasing DM vector, which is independent on the chain length (within the used numerical accuracy). By increasing the DM vector for  $D > D_c$ , the gap opens again in finite

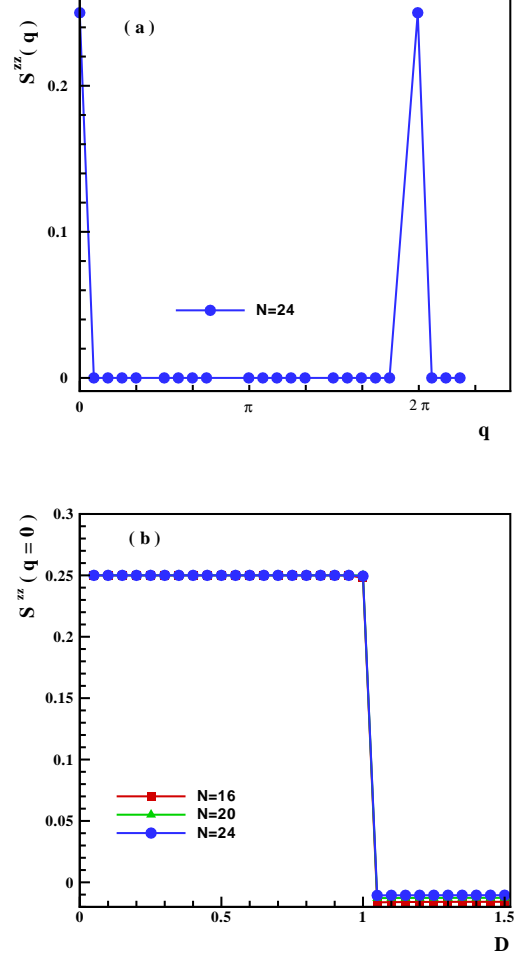


FIG. 2: a) The spin structure factor  $S^{zz}(q)$  as a function of  $q$  for FM Ising chain with DM interaction ( $J = -1.0$  and  $N = 24$ ). b) The spin structure factor  $S^{zz}(q = 0)$  as a function of the DM interaction  $D$  for FM Ising chain ( $J = -1.0$ ) including different chain lengths  $N = 16, 20, 24$ .

chains, but by extrapolating finite size results to  $N \rightarrow \infty$ , we found that there is no gap in the spectrum. That is in agreement with the transformed Hamiltonian results (Eq. 2). Hence there are two gapped and gapless phases in the ground state phase diagram.

To study the magnetic order of the ground state of the system, we have implemented the Lanczos algorithm on finite chains to calculate the lowest eigenstate. The symmetry breaking cannot occur in finite size systems, thus instead of the magnetization,  $M^z = \frac{1}{N} \sum_j \langle S_j^z \rangle$ , we focus on the spin-spin correlation functions. The static spin structure factor at momentum  $q$  is defined as

$$S^{zz}(q) = \frac{1}{N} \sum_n e^{iqn} \langle S_j^z S_{j+n}^z \rangle. \quad (3)$$

It is known that the spin structure factors give us deeper insight into the characteristics of the ground state. The

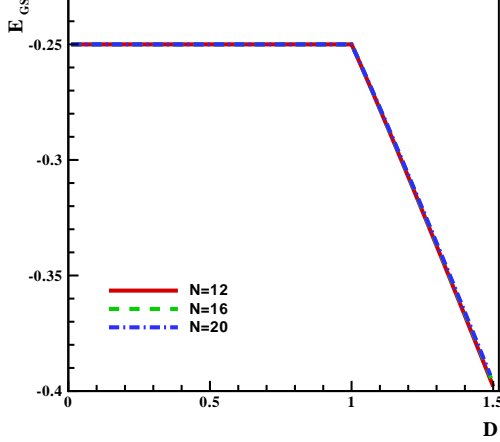


FIG. 3: The numerical results on the ground state energy (normalized by  $N$ ) of a FM Ising model with DM interaction as a function of  $D$  for different chain lengths  $N = 12, 16, 20$  ( $|J| = 1.0$ ).

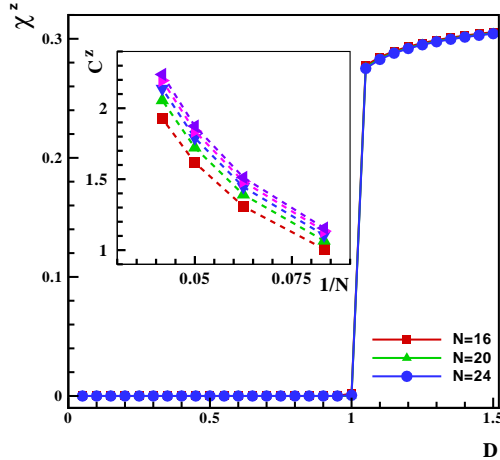


FIG. 4: The spiral order parameter as a function of the DM vector for the FM Ising chain ( $J = -1.0$ ). Inset shows the spiral correlation function,  $C^z$ , as a function of the  $1/N$  for different values of the DM vector:  $D = 1.1, 1.2, 1.3, 1.4, 1.5$ .

$D$ -dependency of the spin structure factor,  $S^{zz}(q = 0)$ , is qualitatively the same as the uniform magnetization,  $M^z$ .

In Fig.2(a) we have plotted the spin structure factor,  $S^{zz}(q)$ , as a function of momentum  $q$  for a chain with length  $N = 24$  and different values of the DM vector in the region  $D < D_c$ . We found that in this region the function  $S^{zz}(q)$  is independent of the value of  $D$ . It shows that  $S^{zz}(q)$  has a very sharp peak at  $q = 0$ , corresponds to the FM ordering. On the other hand, there is not any peak in the region  $D > D_c$  which confirms that all spins should align in the  $xy$  plane. In Fig.2(b),

we have plotted  $S^{zz}(q = 0)$  as a function of  $D$  for the chain lengths  $N = 16, 20, 24$ . For  $D < D_c$  the spin structure factor,  $S^{zz}(q = 0)$ , is equal to the value 0.25, which shows that the ground state of the system is in the fully polarized FM phase. This quantity is independent of the chains size, therefore the value of the magnetization does not change in the thermodynamic limit  $N \rightarrow \infty$ , and the FM ordering is a true long range order in the region  $D < D_c$ . One of the most interesting predictions of this model is that the magnetization as a function of the DM vector displays a jump for certain parameters. It means that the spontaneous magnetization,  $M^z$ , remains at the saturation value in the region  $D < D_c$ . But at the critical value  $D = D_c$ , the spontaneous magnetization jumps to zero. A rapid increase (or discontinuity) at critical value of the control parameter in the magnetization curve is called the metamagnetic phase transition<sup>20,21</sup>. This phenomena that observed in the ground state phase diagram of the 1D frustrated FM Heisenberg model<sup>22,23</sup>, has defined the phase transition between the FM and AF phases. Surprisingly, however, we find that the metamagnetic phase transition can be observed between the FM and spiral phases in the 1D ferromagnetic spin-1/2 Ising model with DM interaction. In following we draw a simple physical picture for this phenomena.

The wave function of the ground state in the absence of the DM interaction has a form  $|\psi_{GS}\rangle = |\uparrow\uparrow\uparrow\dots\rangle$ . Applying a uniform DM interaction on the FM state  $|\psi_{GS}\rangle$  yields

$$\sum_j \mathbf{D} \cdot (\mathbf{S}_j \times \mathbf{S}_{j+1}) |\psi_{GS}\rangle = 0, \quad (4)$$

which shows that in the presence of a DM interaction the ground state is fully polarized and does not change up to the critical value,  $D_c$ . The system is fully FM in  $0 \leq D < D_c$ , and lies in the subspace  $S_{tot} = N/2$  with two-times degeneracy. But it becomes an incommensurate state for  $D > D_c$ , where the energy gap is strongly suppressed. At the critical point, two distinct configurations with the energy  $E_{GS} = -\frac{1}{4}N|J|$  are the ground states, where one is fully polarized in  $z$  direction. In Fig.3, we have plotted the Lanczos results on the ground state energy per sites as a function of  $D$  for the chain lengths  $N = 12, 16, 20$ . As we expected in the region of  $D < D_c$  the energy per spin of the ground state has the constant value  $-0.25$  and independent of the DM interaction ( $E_{GS}/N = -|J|/4$ ).

On the other hand, we have also computed numerically the transverse spin structure factors ( $S^{xx}(q), S^{yy}(q)$ ) for different values of DM vector. Due to symmetry  $S^{xx}(q)$  is the same as  $S^{yy}(q)$ . We found that for the values of the DM vector  $D < D_c$ ,  $S^{xx}(q) = S^{yy}(q) = 0$  in well agreement with the saturated ferromagnetic phase in the  $z$  direction. In the region  $D > D_c$ , the transverse spin structures showed two peaks at  $q = \frac{\pi}{2}, \frac{3\pi}{2}$ , which is a justification of the spiral order<sup>15</sup>. It is showed that the DM interaction can induce the spiral phase in the ground state phase diagram of the spin systems<sup>24</sup>, which

is characterized by the nonzero value of the spirality

$$\chi^z = \frac{1}{N} \sum_j \langle (\mathbf{S}_j \times \mathbf{S}_{j+1})^z \rangle. \quad (5)$$

One should note that there are two different types of the spiral ordered phases, gapped and gapless<sup>25,26</sup>. Therefore, the definition of the spiral correlation function as

$$C^z = \sum_{n=1}^N \langle \chi_j^z \chi_{j+n}^z \rangle, \quad (6)$$

provides further insight into the nature of different phases. In Fig.4, we have presented results of these calculations for Ising chains with different lengths  $N = 16, 20, 24$ . In complete agreement on the results of magnetization, the spirality in the FM Ising chain shows a plateau in zero value at  $D < D_c$ . Which confirms that there is no spiral long range order in the mentioned regime and the ground state is in the saturated FM phase. The spirality remains close to zero value in the region  $D < D_c$ , but at the critical point, it jumps to a non-zero value. Which is also an indication of the metamagnetic quantum phase transition that occurs only in the case of FM Ising chains. The inset of the Fig.4, shows the spiral correlation function,  $C^z$ , as a function of the  $1/N$  for different values of the DM vector. It shows that the spirality remains non zero in the thermodynamic limit for  $D > D_c$ , that corresponds to the spiral long range order in the  $xy$  plane.

### III. VARIATIONAL MATRIX PRODUCT STATES APPROACH

The matrix product state is defined as<sup>27,28</sup>

$$|\Psi\rangle = \text{Tr}(g_1 \cdot g_2 \cdots g_N), \quad (7)$$

where the elementary matrix  $g_j$  represents the matrix-state of the  $j$ th spin cell. The size of these elementary matrices depends on the problem. In this paper the simple one dimensional case is considered, i.e.,  $g_j = a_j |\uparrow\rangle_j + b_j |\downarrow\rangle_j$ . Where  $a_j$  and  $b_j$  are probability amplitude for two configuration of the spin at site  $j$ , and  $N$  is the lattice site number. The goal is to determine the ground state energy of the FM Ising spin system with DM interaction. In this respect, the variational energy is obtained by

$$E_{var} = \langle \mathcal{H} \rangle = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \sum_j \frac{\hat{\mathcal{H}}_{j,j+1}}{[G_j \cdot G_{j+1}]}, \quad (8)$$

where  $\langle \Psi | \Psi \rangle = g_1^\dagger \otimes g_1 \cdots g_N^\dagger \otimes g_N = \prod_j G_j$ , and  $G_j$  is defined by  $G_j = g_j^\dagger \otimes g_j = |a_j|^2 + |b_j|^2$ . Here  $\hat{\mathcal{H}}_{j,k} = J \hat{S}_j^z \hat{S}_k^z + \mathbf{D} \cdot \hat{\mathbf{S}}_j \times \hat{\mathbf{S}}_k$ , and  $\hat{S}_j^\alpha = g_j^\dagger \otimes S_j^\alpha g_j$ .

The minimum of the variational energy function corresponds to the ground state energy of the system. Using the normalization condition  $\langle \Psi | \Psi \rangle = 1$ , variational

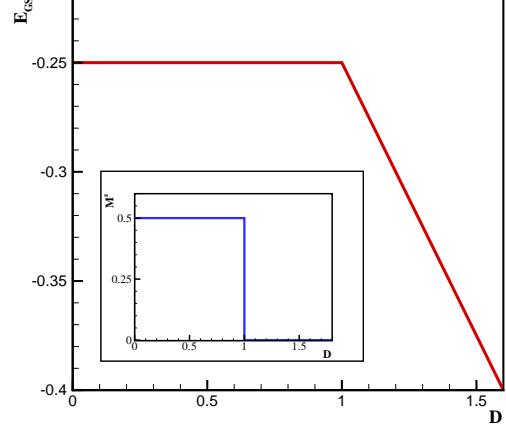


FIG. 5: The ground state energy (normalized by  $N$ ) of FM Ising with DM interaction using the variational matrix product state. Inset shows the spontaneous magnetization  $|M^z|$  as a function of the DM interaction, using the variational matrix product state ( $|J| = 1.0$ ).

parameters can be mapped to  $a_j = \cos(\theta_j) e^{i\varphi_j}$ ,  $b_j = \sin(\theta_j) e^{i\varphi'_j}$ . Therefore one can obtain  $\hat{S}_j^z = \cos(2\theta_j)/2$ ,  $\hat{S}_j^+ = (\hat{S}_j^-)^* = 1/2 \sin(2\theta_j) e^{i\phi_j}$ , where  $\phi_j = (\varphi'_j - \varphi_j)$ . By choosing  $\mathbf{D} = D\hat{z}$ , it is easily found that

$$E_{var} = \frac{1}{4} \sum_j [J \cos(2\theta_j) \cos(2\theta_{j+1}) + D \sin(2\theta_j) \sin(2\theta_{j+1}) \sin(\phi_j - \phi_{j+1})]. \quad (9)$$

By minimizing the above equation, the ground state energy ( $E_{GS}$ ) in the FM case  $J < 0$  shall be achieved. One can show that the ground state energy has the constant value, i.e.  $E_{GS} = -N|J|/4$  for  $D < |J|$ , and it behaves almost linearly for  $D > |J|$  as  $E_{GS} = -ND/4$  (please see the Fig.5).

The magnetization can be written as  $M^z = \sum_j \cos(2\theta_j)/(2N)$ , thus by considering the minimized variational parameters it follows the metamagnetic phase transition curve which has shown in the inset of the Fig.5, where  $|M^z| = 0.5$  at  $D < |J|$  and zero for the  $D > |J|$ . Also the spirality is given by

$$\chi^z = \frac{1}{4N} \sum_j \sin(2\theta_j) \sin(2\theta_{j+1}) \sin(\phi_j - \phi_{j+1}), \quad (10)$$

where using above results, one can obtain  $\chi^z = 0$  for the  $D < |J|$ , and  $|\chi^z| = 0.25$  for  $D > |J|$ .

### IV. SUMMARY AND CONCLUSION

In this paper the elementary excitations and the magnetic ground state phase diagram of the 1D spin-1/2 FM

Ising model with the Dzyaloshinskii-Moriya interaction have been thoroughly investigated by numerical tools and variational schemes. Using the analytical and numerical approaches, we have shown that there are two different phases in the zero-temperature phase diagram of the model. To provide a physical picture of the ground state phase diagram of the model, by a redefinition of the spin variables the model is mapped onto an XXZ Heisenberg chain. Where the anisotropy parameter is related to the DM vector, and identified a commensurate-incommensurate (C-IC) quantum phase transition between the gapped and gapless phases. The numerical experiment with high accuracy, has shown that in the ground state phase diagram of the FM chain with DM interaction, there is only one fully polarized FM phase below the critical value:  $D_c = |J|$ . However at the critical value, a metamagnetic phase transition occurs to the spiral gapless phase. Moreover, we used a variational method for evaluating ground state energy. By considering 1D simple matrix product state, the zero temperature energy diagram of the ferromagnetic Ising chain with DM interaction has been obtained. Our data shows the sud-

den jumping in the magnetization and spirality curves at  $D_c = |J|$ .

Based on the results we conclude that properties of the FM and AF Ising spin-1/2 chains with the uniform DM interaction are very different. In principle, the ground state phase diagram of the FM chain consists of two phases which are gapped and gapless. In the case of FM chains, for  $D < D_c$ , there is only one saturated FM phase and at the critical value,  $D_c$ , a metamagnetic phase transition occurs to the spiral phase.

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- <sup>1</sup> P. Pfeuty, Ann. Phys. **57**, 79 (1970).
  - <sup>2</sup> I. E. Dzyaloshinskii, J. Phys. Chem. Solids **4**, 241 (1958).
  - <sup>3</sup> T. Moriya, Phys. Rev. Lett. **4**, 288 (1960).
  - <sup>4</sup> D. C. Dender et al., Phys. Rev. Lett. **79**, 1750 (1997).
  - <sup>5</sup> J. Sirker, A. Weibe, O. P. Sushkov, Europhys. Lett. **68**, 275 (2004); J. Phys. Soc. Jpn, Suppl. **74**, 129 (2005).
  - <sup>6</sup> T. Sakai, H. Shiba, J. Phys. Soc. Jpn **63**, 867 (1994).
  - <sup>7</sup> G. Chaboussant et al., Eur. Phys. J. B **6**, 167 (1998).
  - <sup>8</sup> H. Kageyama et al., Phys. Rev. Lett. **82**, 3168 (1999).
  - <sup>9</sup> O. Cepas et al., Phys. Rev. Lett. **87**, 167205 (2001).
  - <sup>10</sup> M. Jaime et al., Phys. Rev. Lett. **93**, 087203 (2004).
  - <sup>11</sup> A. Zheludev et al., Phys. Rev. B **59**, 11432 (1999).
  - <sup>12</sup> Oleg Derzhko, Taras Verkholyak, Taras Krokhmal'skii, and Helmut Buttner, Phys. Rev. B **73**, 214407 (2006).
  - <sup>13</sup> U. Schotte et al., J. Phys.: Condens. Matter **10**, 6391 (1998).
  - <sup>14</sup> M. Oshikawa, I. Affleck, Phys. Rev. Lett. **79**, 2883 (1997); Phys. Rev. B **60**, 1038 (1999).
  - <sup>15</sup> R. Jafari, M. Kargarian, A. Langari and M. Siahatgar, Phys. Rev. B **78**, 214414 (2008).
  - <sup>16</sup> F. C. Alcaraz and W. F. Wreszinski, J. Stat. Phys. **58**, 45 (1990).
  - <sup>17</sup> T. A. Kaplan, Z. Phys. B **49**, 313 (1983).
  - <sup>18</sup> H. A. Bethe, Z. Phys. **77**, 205 (1931).
  - <sup>19</sup> M. Takahashi, *Thermodynamics of one-dimensional solvable models*, (Cambridge: Cambridge University Press) (1999).
  - <sup>20</sup> A. Ito et al., J. of Magnetism and Magnetic Materials **104-107**, 1635 (1992).
  - <sup>21</sup> K. Kaczmarek et al., J. of Magnetism and Magnetic Materials **147**, 81 (1995).
  - <sup>22</sup> G. Gerhardt et al., Phys. Rev. B **57**, 11504 (1998).
  - <sup>23</sup> S. Mahdavi, J. Phys.: Condens. Matter **20**, 335230 (2008).
  - <sup>24</sup> S. Mahdavi, M. R. Soltani and A. A. Masoudi, Eur. Phys. J. B **62**, 215 (2008).
  - <sup>25</sup> M. Kaburagi, H. Kawamura, T. Hikihara, J. Phys. Soc. Jpn **68**, 3185 (1999).
  - <sup>26</sup> T. Hikihara et al., J. Phys. Soc. Jpn **69**, 259 (2000).
  - <sup>27</sup> A. Klumper et al., J. Phys. A **24**, L955 (1991); Z. Phys. B **87**, 281 (1992); Europhys. Lett. **24**, 293 (1993).
  - <sup>28</sup> M. Fannes, B. Nachtergaele, and R. F. Werner, Europhys. Lett. **10**, 633 (1989).